Experimental Mathematics: High-Performance Computing Meets Pure Mathematics

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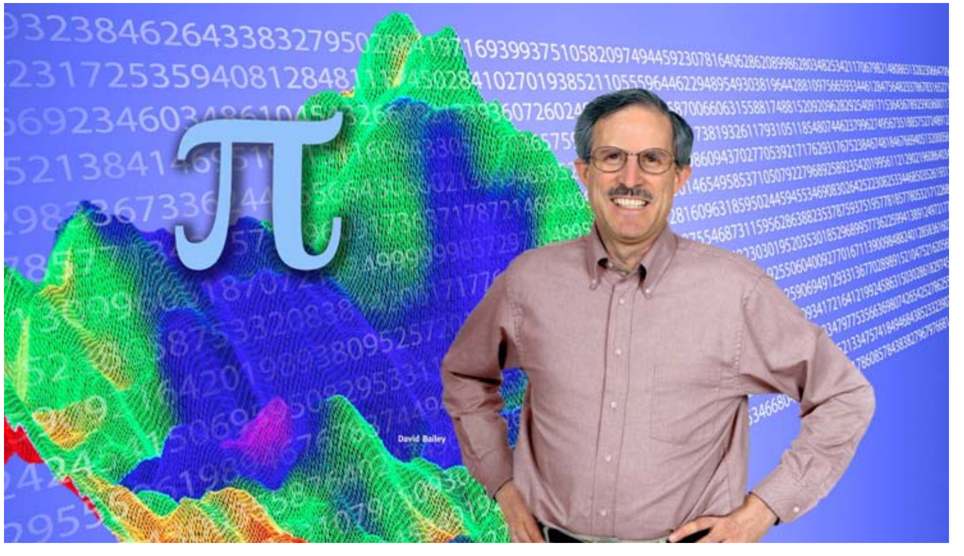


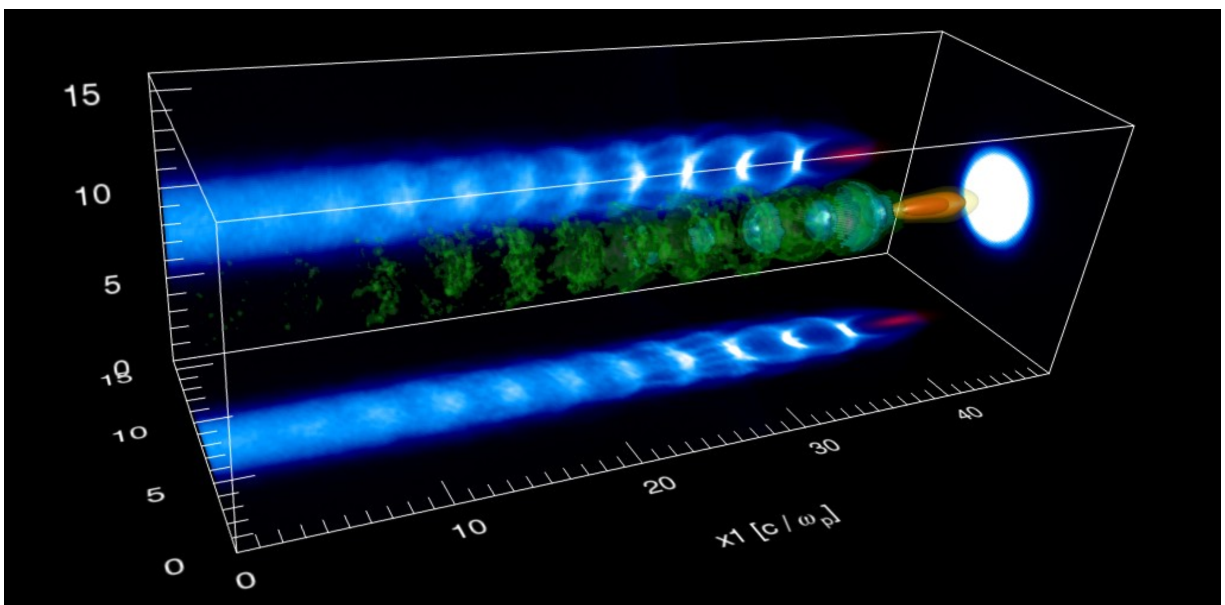
"All truths are easy to understand once they are discovered; the point is to discover them." – Galileo Galilei

The NERSC Computer Center at the Berkeley Laboratory

- Seaborg: 6656-CPU IBM P3 system, 10 Tflop/s peak, 7.8 Tbye memory.
- Bassi: 976-CPU IBM P5 system, 6.7 Tflop/s peak, 3.5 Tbyte memory.
- Franklin (to be installed in early 2007): 9672 dual-core Opteron CPUs, 100 Tflop/s peak, 77 Tbyte memory.

Computations at NERSC: Accelerator Physics

- 3D simulations (such as ORIRIS shown below) have helped experimenters produce 100 MeV beams with significantly improved beam quality.
- Computations involve both dense and sparse linear algebra.
- Presently using 2 million CPU-hours annually.
- Future needs: at least 10 million CPU-hours annually.



Graphic: R. A. Fonseca (IST Portugal), F. S. Tsung (UCLA), and S. Deng (USC)

Climate Modeling

Characteristics:

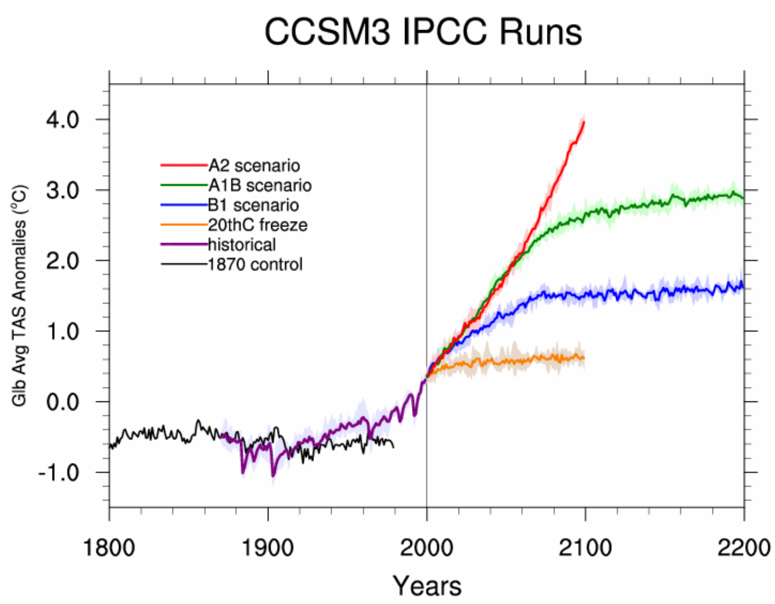
- Hydrodynamics, radiation transfer, thermodynamics, chemical reactions.
- Large finite difference methods, on regular spatial grids.
- Short- to medium-length FFTs are used, although these may be replaced in future.

Current state-of-the-art:

- Atmosphere: 1.4 horizontal deg spacing, with 26 vertical layers.
- Ocean: 1 degree spacing, with 40 vertical layers.
- Currently one simulated day requires 140 seconds on 208 CPUs.

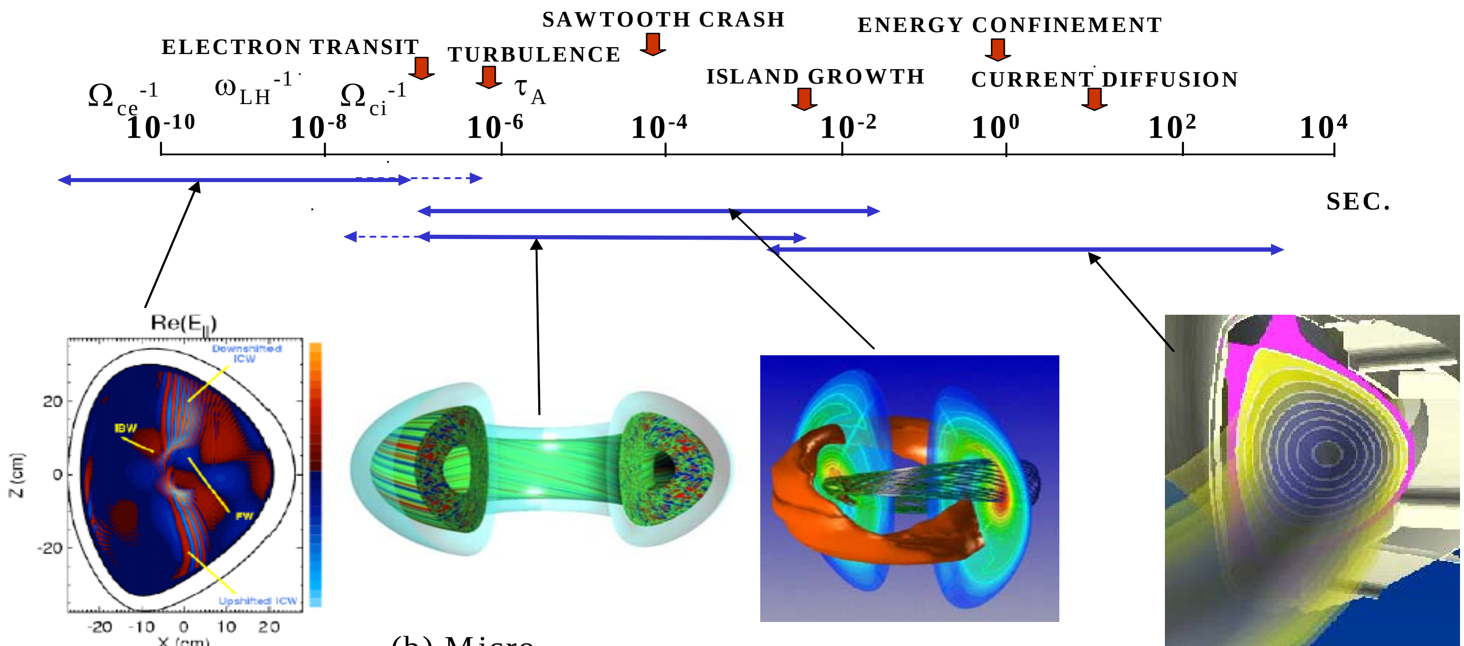
Future requirements:

- 800-1000X current requirements.



Graphic: G. Meehl, J. Arblaster, et al (NCAR)

Fusion Reactor Simulations



(a) RF codes

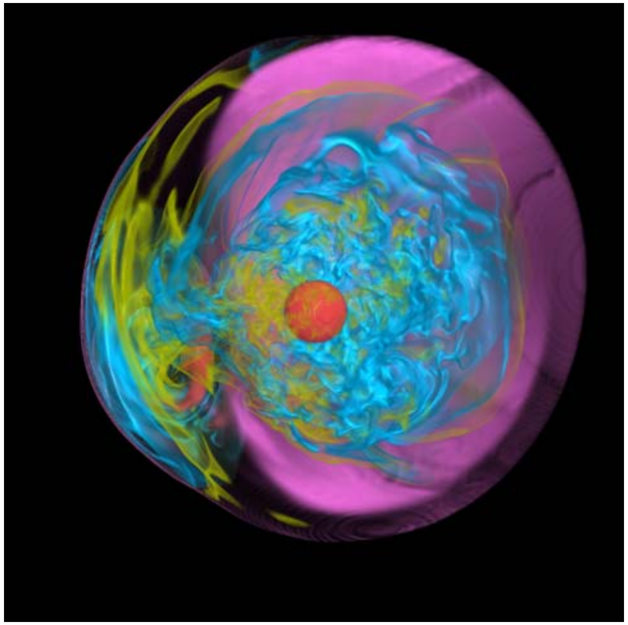
(b) Micro-turbulence codes

(c) Extended-MHD codes

(d) Transport Codes

- Regular and irregular access computations. Graphic: S. Jardin, et al (PPPL)
- Adaptive mesh refinement.
- Advanced nonlinear solvers for stiff PDEs.
- Current: 230 Gbyte memory, 1.3 hours on 1 Tflop/s system (larger problems require 8 hours).
- Future: 576 Tbyte memory, 160 hours on 1 Pflop/s system.

Astrophysics Simulation and Data Analysis



- Multi-physics and multi-scale phenomena.
- Large dynamic range in time and length.
- Requires adaptive mesh refinement.
- Dense linear algebra.
- FFTs and spherical harmonic transforms.

Supernova simulation:

- Future 3-D model calculations will require 1,000,000 CPU-hours per run, on 100 Tflop/s peak system.

Graphic: T. Mezzacappa, J. Blondin, K.-L. Ma, et al (ORNL)

Analysis of cosmic microwave background data:

WMAP (now)	3×10^{21} flops, 16 Tbyte mem
PLANCK (2007)	2×10^{24} flops, 1.6 Pbyte mem
CMBpol (2015)	1×10^{27} flops, 1 Ebyte mem

Characteristics of 21st Century Scientific Computing

- Advanced algorithms, data structures and computational techniques:
  - FFTs.
  - Dense and sparse linear algebra.
  - Iterative solvers.
  - Multigrid.
  - Dynamic data structures.
  - Adaptive mesh refinement.
  - Sophisticated computer graphics and visualization facilities.
  - Large-scale data management facilities.
- State-of-the-art calculations require highly parallel computers:
  - Enormous computational requirements are common.
  - 1000+ CPUs are used in many calculations.
  - Sophisticated parallelization techniques are often required.
- A pragmatic attitude prevails: "If it works, use it."
  - Several widely used numeric algorithms lack formal proofs.

Experimental Mathematics

"Experimental mathematics" means the application of modern computer technology in mathematical research – a merger of computer science and mathematics:

- Gaining insight and intuition.
- Discovering new patterns and relationships.
- Studying underlying principles using graphics and visualization.
- Testing (and often falsifying) conjectures.
- Exploring a result to see if it is worth formal proof.
- Suggesting approaches for formal proof.
- Performing derivations (and checking hand derivations).
- Confirming analytically derived results.

Mathematics is a latecomer to the world of scientific computing, but with the recent advent of powerful mathematical software, it is rapidly gaining ground on fields such as physics and chemistry.

Computational Methods Used in Experimental Math

- High-precision computation (typically hundreds of digits or more).
- PSLQ and other integer relation finding algorithms.
- Symbolic computation.
- Fast Fourier transforms (FFTs).
- Linear and polynomial regression.
- Dense and sparse linear algebra.
- Evaluation of definite integrals and infinite series sums.
- Highly parallel computing.
- Sophisticated computer graphics and visualization facilities.

Except for the first three, all are staples of modern high-performance scientific computing.

Some Supercomputer-Class Experimental Math Computations

Identification of B_4, the fourth bifurcation point of the logistic iteration.

- Integer relation of size 121; 10,000-digit arithmetic; 25 hours CPU time.

Identification of Euler-zeta sums.

- Hundreds of integer relation problems of size 145; 5,000-digit arithmetic; many hours CPU time.

Finding relation involving root of Lehmer's polynomial.

- Integer relation of size 125; 50,000-digit arithmetic; 16 hours on 64 CPUs.

Numerical verification of a mathematical physics integral identity.

- 1-D quadrature calculation; 20,000-digit arithmetic; 45 min on 1024 CPUs.

Numerical evaluation of Ising theory integrals.

- 3-D quadrature of a very complicated function; 500-digit arithmetic;18 hours on 256 CPUs.

Ref: Papers by D. H. Bailey, D. Broadhurst, J. M. Borwein, R. E. Crandall and R. Girgensohn.

LBNL’s High-Precision Software (ARPREC and QD)

- Low-level routines written in C++.
- C++ and F-90 translation modules permit use with existing programs with only minor code changes.
- Double-double (32 digits), quad-double, (64 digits) and arbitrary precision (>64 digits) available.
- Special routines for extra-high precision (>1000 dig).
- Includes common math functions: sqrt, cos, exp, etc.
- PSLQ, root finding, numerical integration.
- An interactive “Experimental Mathematician’s Toolkit” employing this software is also available.

Available at: **`http://www.experimentalmath.info`**

The PSLQ Integer Relation Algorithm

Let (x_n) be a vector of real numbers. An integer relation algorithm finds integers (a_n) such that

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0$$

At the present time, the PSLQ algorithm of mathematician-sculptor Helaman Ferguson is the best-known integer relation algorithm. PSLQ was named one of ten “algorithms of the century” by *Computing in Science and Engineering*.

High-precision arithmetic software is required: at least d x n digits, where d is the size (in digits) of the largest of the integers a_k.

Refs:

1. H. R. P. Ferguson, D. H. Bailey and S. Arno, “Analysis of PSLQ, An Integer Relation Finding Algorithm,” Mathematics of Computation, vol. 68, no. 225 (Jan 1999), pg. 351-369.
2. D. H. Bailey and D. J. Broadhurst, “Parallel Integer Relation Detection: Techniques and Applications,” Mathematics of Computation, vol. 70, no. 236 (Oct 2000), pg. 1719-1736.

The BBP Formula for Pi

In 1996, a computer program running the PSLQ algorithm discovered this formula for pi:

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right)$$

This formula permits one to directly calculate binary or hexadecimal (base-16) digits of pi beginning at an arbitrary starting position n, without needing to calculate any of the first n-1 digits.

This formula is now used in the G95 compiler.

Ref: D. H. Bailey, P. B. Borwein and S. Plouffe, “On the Rapid Computation of Various Polylogarithmic Constants,” Mathematics of Computation, vol. 66, no. 218 (Apr 1997), pg. 903-913.

Some Other Similar BBP-Type Identities

$$\pi^2 = \frac{1}{8}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{144}{(6k+1)^2}-\frac{216}{(6k+2)^2}-\frac{72}{(6k+3)^2}-\frac{54}{(6k+4)^2}+\frac{9}{(6k+5)^2}\right)$$

$$\pi^2 = \frac{2}{27}\sum_{k=0}^{\infty}\frac{1}{729^k}\left(\frac{243}{(12k+1)^2}-\frac{405}{(12k+2)^2}-\frac{81}{(12k+4)^2}-\frac{27}{(12k+5)^2}\right.$$
$$\left.-\frac{72}{(12k+6)^2}-\frac{9}{(12k+7)^2}-\frac{9}{(12k+8)^2}-\frac{5}{(12k+10)^2}+\frac{1}{(12k+11)^2}\right)$$

$$\zeta(3) = \frac{1}{1792}\sum_{k=0}^{\infty}\frac{1}{2^{12k}}\left(\frac{6144}{(24k+1)^3}-\frac{43008}{(24k+2)^3}+\frac{24576}{(24k+3)^3}+\frac{30720}{(24k+4)^3}\right.$$
$$-\frac{1536}{(24k+5)^3}+\frac{3072}{(24k+6)^3}+\frac{768}{(24k+7)^3}-\frac{3072}{(24k+9)^3}-\frac{2688}{(24k+10)^3}$$
$$-\frac{192}{(24k+11)^3}-\frac{1536}{(24k+12)^3}-\frac{96}{(24k+13)^3}-\frac{672}{(24k+14)^3}-\frac{384}{(24k+15)^3}$$
$$+\frac{24}{(24k+17)^3}+\frac{48}{(24k+18)^3}-\frac{12}{(24k+19)^3}+\frac{120}{(24k+20)^3}+\frac{48}{(24k+21)^3}$$
$$\left.-\frac{42}{(24k+22)^3}+\frac{3}{(24k+23)^3}\right)$$

$$\frac{25}{2}\log\left(\frac{781}{256}\left(\frac{57-5\sqrt{5}}{57+5\sqrt{5}}\right)^{\sqrt{5}}\right) = \sum_{k=0}^{\infty}\frac{1}{5^{5k}}\left(\frac{5}{5k+2}+\frac{1}{5k+3}\right)$$

Ref: Papers by D. H. Bailey, P. B. Borwein, S. Plouffe, D. Broadhurst and R. E. Crandall.

A Connection Between BBP Formulas and Normality

A real number x is "b-normal" or "normal base b" if every m-long string of digits appears in the base-b expansion of x with frequency $1/b^m$ (i.e. with the frequency expected in a random sequence). A long-standing unsolved problem of mathematics is to prove that pi, e, log(2), sqrt(2), etc are normal (to any base).

Let {t} denote the fractional part of t, and consider the sequence $x_0 = 0$, and

$$x_n = \left\{2x_{n-1} + \frac{1}{n}\right\}$$

Theorem: log(2) is 2-normal if and only if this sequence is equidistributed in the unit interval.

In a similar vein, consider the sequence $x_0 = 0$, and

$$x_n = \left\{16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21}\right\}$$

Theorem: Pi is 2-normal if and only if this sequence is equidistributed in the unit interval.

Ref: D. H. Bailey and R. E. Crandall, “On the Random Character of Fundamental Constant Expansions,” Experimental Mathematics, vol. 10, no. 2 (Jun 2001), pg. 175-190.

A Class of Provably Normal Constants

We have also shown that an infinite class of mathematical constants is normal, including

$$\alpha_{2,3} = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}}$$
$$= 0.041883680831502985071252898624571682426096\ldots_{10}$$
$$= \texttt{0.0AB8E38F684BDA12F684BF35BA781948B0FCD6E9E0}\ldots_{16}$$

This was proven 2-normal by Stoneham in 1971, but we have extended this result to the case where (2,3) are any pair (p,q) of relatively prime integers. We also extended to an uncountably infinite class [here r_k is the k-th bit of r]:

$$\alpha_{2,3}(r) = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k + r_k}}$$

Ref: D. H. Bailey and R. E. Crandall, "Random Generators and Normal Numbers," Experimental Mathematics, vol. 11, no. 4 (2002), pg. 527-546.

Normal Numbers as Pseudorandom Generators

An effective and efficient pseudo-random number generator can be formulated based on the binary digits of $\alpha_{2,3}$, as follows:

First select a starting index a between $3^{33} + 100 = 5.559 \times 10^{15}$ and $2^{53} = 9.007 \times 10^{15}$. The value of a can be thought of as the "seed" of the generator. Calculate

$$z_0 = (2^{a-3^{33}} \cdot \lfloor 3^{33}/2 \rfloor) \bmod 3^{33}$$

Successive iterates can be generated as

$$z_k = (2^{53} \cdot z_{k-1}) \bmod 3^{33}$$

Normalizing this sequence by 3^{33} produces a sequence of 64-bit IEEE floats in the unit interval, which are in fact successive 53-bit sections of the binary digits of $a_{2,3}$ (within a certain range).

The resulting scheme runs at rate equivalent to that of a conventional linear-congruential pseudorandom generator.

Recent PSLQ Results: Apery-Like Sum Identities

The following identities were recently found using integer relation methods:

$$\zeta(5) = 2\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}} - \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2},$$

$$\zeta(7) = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}$$

$$\zeta(9) = \frac{9}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^9\binom{2k}{k}} - \frac{5}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2} + 5\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}$$
$$+\frac{45}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^6} - \frac{25}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\sum_{j=1}^{k-1}\frac{1}{j^2},$$

$$\sum_{n=0}^{\infty}\zeta(4n+3)x^{4n} = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}(1-x^4/k^4)}\prod_{m=1}^{k-1}\left(\frac{1+4x^4/m^4}{1-x^4/m^4}\right)$$

$$\sum_{n=0}^{\infty}\zeta(2n+2)x^{2n} = 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}\left(1-x^2/k^2\right)}\prod_{m=1}^{k-1}\left(\frac{1-4x^2/m^2}{1-x^2/m^2}\right)$$

Ref: D. H. Bailey, J. M. Borwein and D. M. Bradley, “Experimental Determination of Apery-Like Identities for Zeta(2n+2),” Experimental Mathematics, to appear.

Tanh-Sinh Numerical Quadrature

Given f(x) defined on (-1,1), substitute x = g(t), where g(t) = tanh(sinh t):

$$\int_{-1}^{1} f(x)\,dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \;\approx\; h\sum_{-N}^{N} w_j f(x_j)$$

where $x_j = g(hj)$ and $w_j = g'(hj)$.

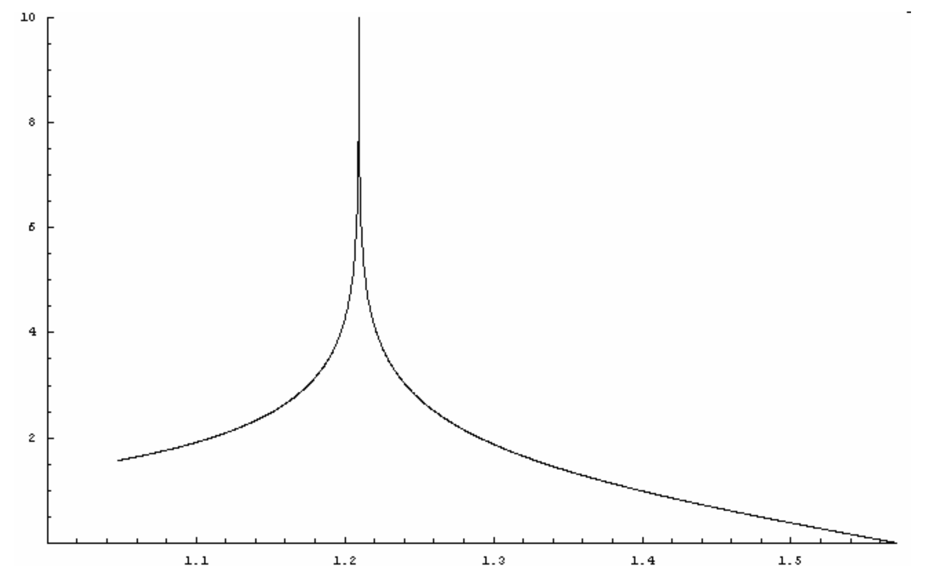
Because g'(t) goes to zero rapidly for large t, the product f(g(t)) g'(t) usually is a nice bell-shaped function, even in cases where f(x) has a vertical derivative or blow-up singularity at an endpoint. For such functions, the Euler-Maclaurin formula implies that the error in this approximation decreases very rapidly with h.

This scheme often achieves quadratic convergence – reducing h by half produces twice as many correct digits.

Application of High-Precision Tanh-Sinh Quadrature

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt$$
$$\stackrel{?}{=} \sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]$$

This arises from analysis of volumes of ideal tetrahedra in hyperbolic space. This "identity" has now been verified numerically to 20,000 digits, but no proof is known.



Ref: D.H. Bailey, J.M. Borwein, V. Kapoor and E. Weisstein, “Ten Problems in Experimental Mathematics,” Am. Math. Monthly, Jun 2006.

Box Integrals

Spurred by a question posed in Jan 2006 by Luis Goddyn of SFU, we examined some integrals of the form:

$$B_n(s) = \int_0^1 \cdots \int_0^1 \left(r_1^2 + \ldots + r_n^2\right)^{s/2} \, dr_1 \cdots dr_n$$

The following evaluations are now known:

$$\begin{aligned}
B_1(1) &= \frac{1}{2} \\
B_2(1) &= \frac{\sqrt{2}}{3} + \frac{1}{3} \log\left(\sqrt{2} + 1\right) \\
B_3(1) &= \frac{\sqrt{3}}{4} + \frac{1}{2} \log\left(2 + \sqrt{3}\right) - \frac{\pi}{24} \\
B_4(1) &= \frac{2}{5} + \frac{7}{20}\pi\sqrt{2} - \frac{1}{20}\pi \log\left(1 + \sqrt{2}\right) + \log(3) - \frac{7}{5}\sqrt{2}\arctan\left(\sqrt{2}\right) + \frac{1}{10}\mathcal{K}_0
\end{aligned}$$

where

$$\mathcal{K}_0 = \int_0^1 \frac{\log(1 + \sqrt{3 + y^2}) - \log(-1 + \sqrt{3 + y^2})}{1 + y^2} \, dy$$

Ref: D. H. Bailey, J. M. Borwein and R. E. Crandall, “Box Integrals,” Journal of Computational and Applied Mathematics, to appear.

Ising Integrals

We recently applied our methods to study some integrals that arise in the Ising theory of mathematical physics:

$$C_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2}\frac{du_1}{u_1}\cdots\frac{du_n}{u_n}$$

$$D_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2}\frac{du_1}{u_1}\cdots\frac{du_n}{u_n}$$

$$E_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2 \frac{du_1}{u_1}\cdots\frac{du_n}{u_n}$$

Computing and Evaluating C_n

Richard Crandall showed that the multi-dimensional C_n integrals can be transformed to 1-D integrals:

$$C_n = \frac{2^n}{n!} \int_0^\infty t K_0^n(t) \; dt$$

where K_0 is the modified Bessel function.

We used this formula to compute 500-digit numerical values of various C_n, from which these results and others were found (and subsequently proven):

$$\begin{aligned}
C_1 &= 2 \\
C_2 &= 1 \\
C_3 &= \mathrm{L}_{-3}(2) = \sum_{n \geq 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right) \\
C_4 &= 14\zeta(3)
\end{aligned}$$

Limiting Value of C_n

C_n appear to approach a limit:

$$
\begin{aligned}
C_{10} &= 0.6318800241470122222903508736608028 3\ldots \\
C_{40} &= 0.6304735033783635318699419018590969 4\ldots \\
C_{100} &= 0.6304735033743867961220401927190317 1\ldots \\
C_{200} &= 0.6304735033743867961220401927108789 0\ldots
\end{aligned}
$$

What is this limit? We pasted the first 50 digits of this numerical value into the Inverse Symbolic Calculator tool, available at

`http://oldweb.cecm.sfu.ca/projects/ISC/ISCmain.html`

The result was: $2e^{-2\gamma}$

where gamma denotes Euler's constant. In fact, we have now proven:

$$C_n = 2\,e^{-2\gamma} + \frac{n+4}{2^n}e^{-4\gamma} + \frac{2n^2+23n+57}{3^n \cdot 6}e^{-6\gamma} + \cdots$$

Other Evaluations

$$
\begin{aligned}
D_2 &= 1/3 \\
D_3 &= 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2) \\
D_4 &= 4\pi^2/9 - 1/6 - 7\zeta(3)/2 \\
E_2 &= 6 - 8\log 2 \\
E_3 &= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2 \\
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3 \\
&\quad +16\pi^2\log 2 - 22\pi^2/3 \\
E_5 &\stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2 \\
&\quad +40\pi^2\log^2 2 - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2 \\
&\quad +464\log^2 2 - 40\log 2
\end{aligned}
$$

The Ising Integral E_5

We were able to reduce E_5, which is a 5-D integral, to an extremely complicated 3-D integral (see below).

We computed this integral to 250-digit precision, using a parallel high-precision 3-D quadrature program. Then we used a PSLQ program to discover the evaluation given on the previous page.

$$
\begin{aligned}
E_5 = \int_0^1\int_0^1\int_0^1 & [2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 (-[4(x+1)(xy+1)\log(2)(y^5z^3x^7 - y^4z^2(4(y+1)z+3)x^6 - y^3z((y^2+1)z^2+4(y+\\
& 1)z+5)x^5 + y^2(4y(y+1)z^3+3(y^2+1)z^2+4(y+1)z-1)x^4 + y(z(z^2+4z+5)y^2+4(z^2+1)y+5z+4)x^3 + ((-3z^2-4z+1)y^2-4zy+1)x^2\\
& -(y(5z+4)+4)x-1)] / [(x-1)^3(xy-1)^3(xyz-1)^3] + [3(y-1)^2y^4(z-1)^2z^2(yz-1)^2x^6 + 2y^3z(3(z-1)^2z^3y^5 + z^2(5z^3+3z^2+3z+5)y^4 + (z-1)^2z\\
& (5z^2+16z+5)y^3 + (3z^5+3z^4-22z^3-22z^2+3z+3)y^2 + 3(-2z^4+z^3+2z^2+z-2)y + 3z^3+5z^2+5z+3)x^5 + y^2(7(z-1)^2z^4y^6 - 2z^3(z^3+15z^2\\
& +15z+1)y^5 + 2z^2(-21z^4+6z^3+14z^2+6z-21)y^4 - 2z(z^5-6z^4-27z^3-27z^2-6z+1)y^3 + (7z^6-30z^5+28z^4+54z^3+28z^2-30z+7)y^2 - 2(7z^5\\
& +15z^4-6z^3-6z^2+15z+7)y + 7z^4-2z^3-42z^2-2z+7)x^4 - 2y(z^3(z^3-9z^2-9z+1)y^6 + z^2(7z^4-14z^3-18z^2-14z+7)y^5 + z(7z^5+14z^4+3\\
& z^3+3z^2+14z+7)y^4 + (z^6-14z^5+3z^4+84z^3+3z^2-14z+1)y^3 - 3(3z^5+6z^4-z^3-z^2+6z+3)y^2 - (9z^4+14z^3-14z^2+14z+9)y + z^3+7z^2+7z\\
& +1)x^3 + (z^2(11z^4+6z^3-66z^2+6z+11)y^6 + 2z(5z^5+13z^4-2z^3-2z^2+13z+5)y^5 + (11z^6+26z^5+44z^4-66z^3+44z^2+26z+11)y^4 + (6z^5-4\\
& z^4-66z^3-66z^2-4z+6)y^3 - 2(33z^4+2z^3-22z^2+2z+33)y^2 + (6z^3+26z^2+26z+6)y + 11z^2+10z+11)x^2 - 2(z^2(5z^3+3z^2+3z+5)y^5 + z(22z^4\\
& +5z^3-22z^2+5z+22)y^4 + (5z^5+5z^4-26z^3-26z^2+5z+5)y^3 + (3z^4-22z^3-26z^2-22z+3)y^2 + (3z^3+5z^2+5z+3)y + 5z^2+22z+5)x + 15z^2+2z\\
& +2y(z-1)^2(z+1) + 2y^3(z-1)^2z(z+1) + y^4z^2(15z^2+2z+15) + y^2(15z^4-2z^3-90z^2-2z+15) + 15] / [(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2\\
& (xyz-1)^2] - [4(x+1)(y+1)(yz+1)(-z^2y^4 + 4z(z+1)y^3 + (z^2+1)y^2 - 4(z+1)y + 4x(y^2-1)(y^2z^2-1) + x^2(z^2y^4 - 4z(z+1)y^3 - (z^2+1)y^2\\
& +4(z+1)y+1) - 1)\log(x+1)] / [(x-1)^3x(y-1)^3(yz-1)^3] - [4(y+1)(xy+1)(z+1)(x^2(z^2-4z-1)y^4 + 4x(x+1)(z^2-1)y^3 - (x^2+1)(z^2-4z-1)\\
& y^2 - 4(x+1)(z^2-1)y + z^2-4z-1)\log(xy+1)] / [x(y-1)^3y(xy-1)^3(z-1)^3] - [4(z+1)(yz+1)(x^3y^5z^7 + x^2y^4(4x(y+1)+5)z^6 - xy^3((y^2+\\
& 1)x^2 - 4(y+1)x - 3)z^5 - y^2(4y(y+1)x^3 + 5(y^2+1)x^2 + 4(y+1)x + 1)z^4 + y(y^2x^3 - 4y(y+1)x^2 - 3(y^2+1)x - 4(y+1))z^3 + (5x^2y^2 + y^2 + 4x(y+1)\\
& y+1)z^2 + ((3x+4)y+4)z - 1)\log(xyz+1)] / [xy(z-1)^3z(yz-1)^3(xyz-1)^3])] / [(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2]\\
& dx\,dy\,dz
\end{aligned}
$$

Recursions in Ising Integrals

Consider this 2-parameter class of Ising integrals:

$$C_{n,k} = \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^{k+1}} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

After computing 1000-digit numerical values for all n up to 36 and all k up to 75 (a total of 2660 individual quadrature calculations), we discovered (using PSLQ) linear relations in the rows of this array. For example, when n = 3:

$$\begin{aligned}
0 &= C_{3,0} - 84C_{3,2} + 216C_{3,4} \\
0 &= 2C_{3,1} - 69C_{3,3} + 135C_{3,5} \\
0 &= C_{3,2} - 24C_{3,4} + 40C_{3,6} \\
0 &= 32C_{3,3} - 630C_{3,5} + 945C_{3,7} \\
0 &= 125C_{3,4} - 2172C_{3,6} + 3024C_{3,8}
\end{aligned}$$

Similar, but more complicated, recursions were found for larger n (next page).

Experimentally-Found Recursion for n = 24

$$
\begin{aligned}
0 \stackrel{?}{=}\; & C_{24,1} \\
& -1107296298\, C_{24,3} \\
& +1288574336175660\, C_{24,5} \\
& -88962910652291256000\, C_{24,7} \\
& +1211528914846561331193600\, C_{24,9} \\
& -5367185923241422152980553600\, C_{24,11} \\
& +9857686103738772925980190636800\, C_{24,13} \\
& -8476778037073141951236532459008000\, C_{24,15} \\
& +3590120926882411593645052529049600000\, C_{24,17} \\
& -745759114781380983188217871663104000000\, C_{24,19} \\
& +71215552121869985477578381170258739200000\, C_{24,21} \\
& -2649853457247995406113355087174696960000000\, C_{24,23} \\
& +24912519234220575094208313195233280000000000\, C_{24,25}
\end{aligned}
$$

General Recursion Formulas

We were able to find general recursion formulas for each n:

$$
\begin{aligned}
0 &= (k+1)C_{1,k} - (k+2)C_{1,k+2} \\
0 &= (k+1)^2 C_{2,k} - 4(k+2)^2 C_{2,k+2} \\
0 &= (k+1)^3 C_{3,k} - 2(k+2)\left(5(k+2)^2+1\right) C_{3,k+2} \\
&\quad +9(k+2)(k+3)(k+4)C_{3,k+4} \\
0 &= (k+1)^4 C_{4,k} - 4(k+2)^2(5(k+2)^2+3)C_{4,k+2} \\
&\quad +64(k+2)(k+3)^2(k+4)C_{4,k+4} \\
0 &\stackrel{?}{=} (k+1)^5 C_{5,k} - (k+2)\left(35k^4+280k^3+882k^2+1288k+731\right) C_{5,k+2} \\
&\quad +(k+2)(k+3)(k+4)\left(259k^2+1554k+2435\right) C_{5,k+4} \\
&\quad -225(k+2)(k+3)(k+4)(k+5)(k+6)C_{5,k+6} \\
0 &\stackrel{?}{=} (k+1)^6 C_{6,k} - 8(k+2)^2\left(7k^4+56k^3+182k^2+280k+171\right) C_{6,k+2} \\
&\quad +16(k+2)(k+3)^2(k+4)\left(49k^2+294k+500\right) C_{6,k+4} \\
&\quad -2304(k+2)(k+3)(k+4)^2(k+5)(k+6)C_{6,k+6}
\end{aligned}
$$

Compact Recursion Formulas

Let $c_{n,k} = n!\, k!\, 2^{-n}\, C_{n,k}$ and let M be the largest integer in (n+1)/2. We found (using high-precision polynomial regression) that all of these recursions can be written in the compact form

$$\sum_{i=0}^{M} (-1)^i p_{n,i}(k+i+1)\, c_{n,k+2i} = 0$$

for certain relatively simple polynomials $p_{n,i}(x)$. Here are the polynomials for n = 5 and n = 6:

$$\begin{aligned} p_{5,0}(x) &= x^6 \\ p_{5,1}(x) &= 35x^4 + 42x^2 + 3 \\ p_{5,2}(x) &= 259x^2 + 104 \\ p_{5,3}(x) &= 225 \end{aligned}$$

$$\begin{aligned} p_{6,0}(x) &= x^7 \\ p_{6,1}(x) &= x(56x^4 + 112x^2 + 24) \\ p_{6,2}(x) &= x(784x^2 + 944) \\ p_{6,3}(x) &= 2304x \end{aligned}$$

Polynomials $p_{n,i}(x)$ for i = 1,2

n	$i=1$
1	1
2	$4x$
3	$2+10x^2$
4	$x(12+20x^2)$
5	$3+42x^2+35x^4$
6	$x(24+112x^2+56x^4)$
7	$4+108x^2+252x^4+84x^6$
8	$x(40+360x^2+504x^4+120x^6)$
9	$5+220x^2+990x^4+924x^6+165x^8$
10	$x(60+880x^2+2376x^4+1584x^6+220x^8)$
11	$6+390x^2+2860x^4+5148x^6+2574x^8+286x^{10}$
12	$x(84+1820x^2+8008x^4+10296x^6+4004x^8+364x^{10})$
n	$i=2$
3	9
4	$64x$
5	$104+259x^2$
6	$x(944+784x^2)$
7	$816+4752x^2+1974x^4$
8	$x(9024+17520x^2+4368x^4)$
9	$5376+54384x^2+52800x^4+8778x^6$
10	$x(70144+236544x^2+137808x^4+16368x^6)$
11	$32000+492544x^2+830544x^4+322608x^6+28743x^8$
12	$x(481280+2469376x^2+2498496x^4+693264x^6+48048x^8)$

Polynomials $p_{n,i}(x)$ for i = 3,4,5,6

n	$i = 3$
5	225
6	$2304x$
7	$7796 + 12916x^2$
8	$x(94976 + 52480x^2)$
9	$170298 + 625196x^2 + 172810x^4$
10	$x(2409216 + 2949056x^2 + 489280x^4)$
11	$2999076 + 18232188x^2 + 11161436x^4 + 1234948x^6$
12	$x(48354048 + 98000448x^2 + 36003968x^4 + 2846272x^6)$
n	$i = 4$
7	11025
8	$147456x$
9	$851976 + 1057221x^2$
10	$x(13036544 + 5395456x^2)$
11	$39605040 + 106102880x^2 + 21967231x^4$
12	$x(683253760 + 610355200x^2 + 75851776x^4)$
n	$i = 5$
9	893025
10	$14745600x$
11	$129879846 + 128816766x^2$
12	$x(2393358336 + 791691264x^2)$
n	$i = 6$
11	108056025
12	$2123366400x$

Closed Forms for $p_{n,i}(x)$

$$
\begin{aligned}
p_{n,0}(x) &= x^{n+1} \\
p_{n,1}(x) &= \sum_{j=1}^{M} j \binom{n+2}{2j+1} x^{n+1-2j} \\
p_{n,2}(x) &= \sum_{j=1}^{M-1} \frac{j4^{j-1}((2j+3)(n+2)+j+1)}{j+2} \cdot \binom{n+2}{2j+3} x^{n+1-2j}
\end{aligned}
$$

Can we extend these results for i > 2? This is currently under investigation.

For further details, see:

1. D. H. Bailey, J. M. Borwein and R. E. Crandall, “Integrals of the Ising Class,” Journal of Physics A: Mathematical and General, to appear.
2. D. H. Bailey, D. Borwein, J. M. Borwein and R. E. Crandall, “Hypergeometric Forms for Ising-Class Integrals,” Experimental Mathematics, to appear.
3. D. H. Bailey, J. M. Borwein and R. E. Crandall, “Finding General Explicit Formulas for Ising Integral Recursions,” manuscript (work in progress).

Preprints are available at http://crd.lbl.gov/~dhbailey/dhbpapers.

Experimental Math as a Branch of 21st Century Scientific Computing

- Advanced numerical algorithms and computational techniques:
  - High-precision computation (typically hundreds or thousands of digits).
  - PSLQ and other integer relation finding algorithms.
  - Symbolic computation.
  - Fast Fourier transforms (FFTs).
  - Linear and polynomial regression.
  - Dense and sparse linear algebra.
  - Evaluation of definite integrals and infinite series sums.
  - Sophisticated computer graphics and visualization facilities.
- State-of-the-art calculations require highly parallel computers:
  - Enormous computational requirements are common.
  - 1000+ CPUs are used in many calculations.
  - Sophisticated parallelization techniques are often required.
- A pragmatic attitude prevails: “If it works, use it.”
  - Several widely used experimental math algorithms lack formal proofs.

The Appeal of Experimental Math

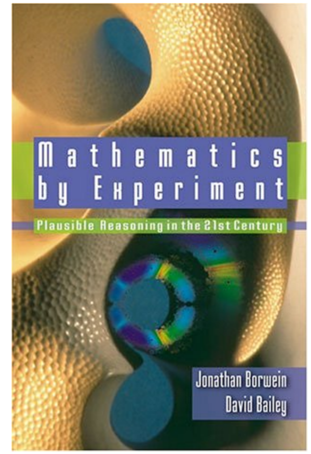
- Experimental math is accessible.
  - Much is readily understandable to persons with only modest mathematical backgrounds.
- Experimental math is multidisciplinary.
  - Computer scientists, numerical analysts, mathematicians and physicists have all made significant contributions.
- Experimental math excites the younger, computer-savvy generation.
  - Students (both in math and computer science) with good programming skills can do real publishable research.
- Experimental math is an excellent tool for student learning.
  - With a few experiments, students can “see” what’s happening.
  - Computer graphics and plots are particularly useful.
  - Student versions of *Mathematica* and *Maple* are now available at very reasonable prices.

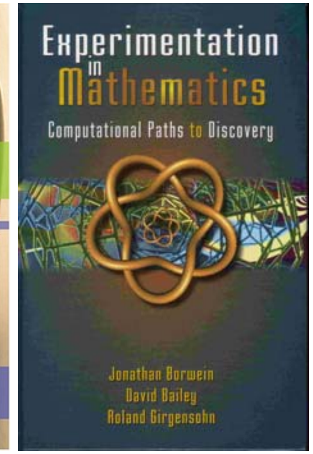
Books on Experimental Mathematics

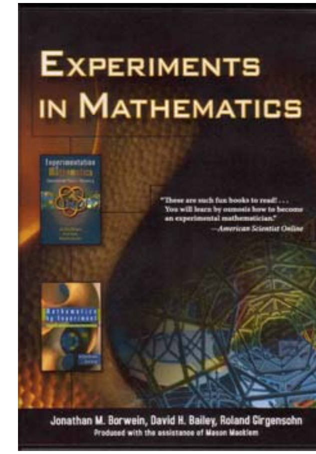
Vol. 1: *Mathematics by Experiment: Plausible Reasoning in the 21st Century*

Vol. 2: *Experiments in Mathematics: Computational Paths to Discovery*

Authors: Jonathan Borwein, DHB and (for vol. 2) Roland Girgensohn.







New: Both books are now available on CD-ROM in a hyperlinked, searchable PDF format. Also, a FREE condensed version is available at: **`http://www.experimentalmath.info`**

Coming soon: *Experimental Mathematics in Action*.
Authors: David Bailey, Jon Borwein, Neil Calder, Roland Girgensohn, Russell Luke and Victor Moll.